ASIA CMD® UPM

VENUE

Seminar Room,
Putra Infoport UPM, 43400
Serdang, Selangor, Malaysia

ORGANIZER

Chemistry Unit
Pusat Asasi Sains Pertanian
Universiti Putra Malaysia

FEES

UPM student : RM 700
UPM staff : RM 1,000
Non-UPM student : RM 1,000
Non-UPM staff : RM 1,200

PAYMENT

Account Name: KIRA KIRA AM UPM
Account No: 8002151963
Bank Name: CIMB Bank
Bank Address: CIMB UPM Branch,
43400 UPM, Serdang, Selangor, MALAYSIA
SWIFT Code: CIBBMYKL
Description: TKS239
Reference: ASIA CMD UPM

24 – 26th FEBRUARY 2020

INVITED SPEAKERS

Prof. Dr. Tamio Oguchi
(Osaka University)
Prof. Dr. Yoshitada Morikawa
(Osaka University)
Prof. Dr. Azizan Ahmad
(Universiti Kebangsaan Malaysia)
Prof. Dr. Hideaki Kasai
(National Institute of Technology Japan and Professor Emeritus of Osaka University)
Prof. Dr. Hiroshi Uyama
(Osaka University)
Assoc.Prof. Dr. Wilson Agerico Dino
(Osaka University)
Dr. Mohd Farid Ismail
(Universiti Putra Malaysia)
Mr. Hassan Ahmoum
(Northeastern University, China)
Prof. Dr. Kazunori Sato
(Osaka University)
Dr. Febdian Rusydi
(Universitas Airlangga)

Dr. Intan Diana Mat Azmi (+601139932833)
Cik Noor Hidayu Aris (+60172048845)

asiacmd2020@gmail.com

Registration Link :
https://form.jotform.com/200138370955454

Deadline Registration : 17th February 2020

ASIA CMD® UPM 2020

INTERNATIONAL SYMPOSIUM AND WORKSHOP ON COMPUTATIONAL MATERIAL DESIGN

The Asia CMD® workshop was first held in Institut Teknologi Bandung (ITB), Indonesia in year 2008. Well-known professors from university Japan are invited to conduct a lecture and hand-on sessions on various quantum simulations techniques. This workshop provide insights on developing new materials to meet the ever-increasing demand for novel materials, and at the same time satisfy the growing public concern for the energy/power consumptions.

Quantum ESPRESSO
HiLAPAW
Machikaneyama (KKR)
STATE-Senri
Gaussian 09

ASIA CMD UPM 2020

Quantum ESPRESSO

An integrated suite of Open-Source computer codes for electronic-structure calculations and materials modelling at the nanoscale. It is based on density-functional theory, plane waves, and pseudopotentials. The main features include: Ground-state calculations, Structural Optimization, Transition states and minimum energy paths, Ab-initio molecular dynamics, Response properties (DFPT), Spectroscopic properties, Quantum Transport & Platforms.

HiLAPW

It is designed to perform band-structure calculations based on the density functional theory (DFT). Its main features include scalarrelativistic spin-polarized calculations within the local (spin) density approximation (LSDA); all-electron self-consistent calculations; total-energy and atomic-force calculations for determining the equilibrium structure and phonons; electron density-of-states (DOS) calculations and electron density and potential function calculations for 2D or 3D drawings.

Machikaneyama (KKR)

It used for first-principles calculation of electronic structures of metals, semiconductors and compounds, in the framework of the local density approximation or generalized gradient approximation (LDA/GGA) of the density functional theory. It is an all-electron method. It does not suffer from any serious truncation errors such as those of the plane-wave cutoff. Moreover AkaiKKR is combined with CPA (coherent potential approximation). Thus it is suitable not only for normal ordered crystals but also for disordered systems such as impurity systems, random substitutional alloys and mixed crystals. Since the method directly calculates the Green's function of the system, it can also provide a good starting point for first-principles linear response theory, many-body theory, and so on.

STATE-senri

It is a first-principles molecular dynamics code based on density functional theory (DFT) using a plane wave basis set and ultrasoft pseudopotentials. STATE was designed to perform band structure, total energy and molecular dynamics calculations on parallel supercomputers. The main features include are Norm-conserving pseudopotentials, LSDA & PBE, LDA+U, Iterative diagonalization, Automatic K-points generation, and etc.

TENTATIVE PROGRAM

Monday 24 February 2020 (Day 1) Seminar Room	
08.00 - 09.15	Registration
09.00 - 09.30	Welcome speech by Director of Center : Prof. Dr. Norihan Arifin Doa recitation : En. Mohd Najib
09.30 - 09.50	Officiating speech
09.50 - 10.00	Photo Session
10.00 - 10.15	Morning tea break
10.15 - 10.35	Prof. Dr. Tamio Oguchi **Introduction to CMD and DFT**
10.35 - 10.50	Prof. Dr. Yoshitada Morikawa **Presentation of academic studies from Osaka University, Japan**
10.50 - 11.10	Prof. Dr. Azizan Ahmad **Review on Application of DFT Calculation on Energy Storage Materials.**
11.10 - 11.40	Prof. Dr. Hideaki Kasai **Branching Reactions in Melanogenesis-Mechanism and Design Guidelines**
11.40 - 12.00	Prof. Dr. Hiroshi Uyama **Reactive Cellulose Nanofibers for High-performance and Functinal Polymers**
12.00 - 12.20	Assoc.Prof. Dr. Wilson Agerico Dino **Surface as a Playground and Foundation for Realizing Designer Materials**
12.20 - 14.00	Lunch break
14.00 - 14.45	Dr. Mohd Farid Ismail **Introduction to linux system** Hand on for Linux command
14.45 - 15.00	Mr. Hassan Ahmoum **Introduction to Quantum espresso**
15.00 - 16.45	Hands on for Quantum espresso
16.45 - 17.00	Tea break
17.00	End the session for Day 1

Tuesday 25 Feb 2020 (Day 2) Computer Lab	
08.00 - 09.15	Prof. Dr. Tamio Oguchi **Introduction to HiLAPAW**
09.15 - 09.30	Refresehment
09.30 - 12.00	Hands on for HiLAPAW (Beginner level)
12.00 -13.00	Interpretation and discussion on HiLAPAW - Case study
13.00 - 14.00	Lunch
14.00 - 15.15	Prof. Dr. Kazunori Sato **Introduction to Machikaneyama (KKR)**
15.15 - 16.45	Hands on for Machikaneyama (KKR)
16.45 - 17.00	Coffee break
17.00 - 18.00	Interpretation and discussion on Machikaneyama (KKR) - Case study
18.00	End of session for Day 2
Wednesday 26 February 2020 (Day 3) Computer Lab	
08.30 – 09.15	Prof. Dr. Yoshitada Morikawa **Introduction to STATE-Senri**
09.15 – 09.30	Refreshement
09.30 – 13.00	Hands on for STATE-Senri
13.00 – 14.00	Lunch
14.00 – 14.30	Dr. Febdian Rusydi **Introduction to Gaussian 09**
14.30 – 15.00	Dr. Mark Lee Wun Fui Hands on for Gaussian 09
15.00 – 16.00	Interpretation and discussion on Gaussian - Case study
16.00 – 16.15	Coffee break
16.15 – 16.45	Awarding certificates
16.45 – 17.00	Closing remarks by Prof. Dr. Yoshitada Morikawa
17.10	End the session